

# Shot-noise control in ac-driven nanoscale conductors

Sébastien Camalet,\* Sigmund Kohler, and Peter Hänggi

*Institut für Physik, Universität Augsburg, Universitätsstraße 1, D-86135 Augsburg, Germany*

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We derive within a time-dependent scattering formalism expressions for both the current through ac-driven nanoscale conductors and its fluctuations. The results for the time-dependent current, its time average, and, above all, the driven shot noise properties assume an explicit and serviceable form by relating the propagator to a non-Hermitian Floquet theory. The driven noise cannot be expressed in terms of transmission probabilities. The results are valid for a driving of arbitrary strength and frequency. The connection with commonly known approximation schemes such as the Tien-Gordon approach or a high-frequency approximation is elucidated together with a discussion of the corresponding validity regimes. Within this formalism, we study the coherent suppression of current and noise caused by properly chosen electromagnetic fields.

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## I. INTRODUCTION

The experimental success in the coherent coupling of quantum dots<sup>1,2,3</sup> has enabled measuring the transport properties of systems with a molecule-like level structure. Recently, further progress in this direction has been attained by the reproducible measurement of currents through molecules which are coupled to metallic leads.<sup>4,5</sup> Together with these experimental achievements, new theoretical interest in the transport properties of such nanoscale systems emerged.<sup>6,7</sup> One particular field of interest is the interplay of the electron transport and excitations by an oscillating gate voltage, a microwave field, or an infrared laser, respectively. Such excitations bear intriguing phenomena like photon-assisted tunneling<sup>3,8,9,10,11,12,13,14,15</sup> and the adiabatic<sup>16,17,18,19</sup> and non-adiabatic<sup>20,21,22,23</sup> pumping of electrons.

A prominent example for the control of quantum dynamics is the so-called coherent destruction of tunneling, i.e., the suppression of the tunneling dynamics of a particle in a double-well potential,<sup>24</sup> in a two-level system,<sup>25</sup> or in a superlattice.<sup>26</sup> Recently, coherent destruction of tunneling has also been found for the dynamics of two interacting electrons in a double quantum dot.<sup>27,28</sup> Moreover, it has been demonstrated that a corresponding transport effect exists: If two leads are attached to the ends of a tunneling system, then a proper driving field can be used to suppress the current even in the presence of a large transport voltage.<sup>29</sup> Moreover, in such a system the corresponding shot noise level *a priori* can be controlled by proper ac fields.<sup>30</sup> Within this work, we provide more details on this noise control scheme and also explore its limitations.

An intuitive description of the electron transport through time-independent mesoscopic systems is provided by the Landauer scattering formula<sup>31</sup> and its various generalizations. Both the average current<sup>32</sup> and the transport noise characteristics<sup>33,34</sup> can be expressed in terms of the quantum transmission coefficients for the respective scattering channels. By contrast, the theory for driven quantum transport is less developed. Scatter-

ing of a single particle by an arbitrary time-dependent potentials has been considered<sup>35,36,37</sup> without relating the resulting transmissions to a current between electron reservoirs. Such a relation is indeed non-trivial since the driving opens inelastic transport channels and, therefore, in contrast to the static case, an *ad hoc* inclusion of the Pauli principle is no longer unique. This gave rise to a discussion about “Pauli blocking factors”.<sup>38,39</sup> In order to avoid such conflicts, one should start out from a many-particle description. In this spirit, within a Green function approach, a *formal* solution for the current through a time-dependent conductor has been presented, e.g., in Refs. 38 and 40 without taking advantage of the full Floquet theory for the wire. Nevertheless in some special cases like, e.g., for conductors consisting of a single level<sup>41,42</sup> or for the scattering by a piecewise constant potential,<sup>9,20</sup> an explicit solution becomes feasible. Moreover, for large driving frequencies, the driving can be treated within a self-consistent perturbation theory.<sup>43,44</sup>

The spectral density of the current fluctuations has been derived for the low-frequency ac conductance<sup>45,46</sup> and the scattering by a slowly time-dependent potential.<sup>47</sup> For arbitrary driving frequencies, the noise has been characterized by its zero-frequency component.<sup>30</sup> A remarkable feature of the current noise in the presence of time-dependent fields is its dependence on the phase of the transmission *amplitudes*.<sup>30,47</sup> By clear contrast, both the noise in the static case<sup>33</sup> and the current in the driven case<sup>30</sup> depend solely on transmission *probabilities*.

Within this work, we *derive* within a Floquet approach explicit expressions for both the current and the noise properties of the electron transport through a driven nanoscale conductor under the influence of time-dependent forces. This generalizes recent approaches since the presented Floquet formalism is applicable to arbitrary periodically driven tight-binding systems and, in particular, is valid for arbitrary driving strength and, as well, extends beyond the adiabatic regime. The dynamics of the electrons is solved by integrating the Heisenberg

equations of motion for the electron creation/annihilation operators in terms of the single-particle propagator. For this propagator, in turn, we provide a solution within a generalized Floquet approach. Such a treatment is valid for effectively non-interacting electrons, i.e., when no strong correlations occur. Disregarding these interactions also implies that the displacement currents are not taken into account entirely. As a consequence, the ac component of the electrical current *inside* the nanoconductor may deviate from the particle current.<sup>33,48</sup>

This paper is organized as follows. After introducing in Sec. II a model for the leads and the conductor under the influence of external fields, we derive in Sec. III for a situation with time-periodic but otherwise arbitrary driving general expressions for the current and its noise and establish a connection to a Floquet eigenvalue equation. In Sec. IV, we consider some special cases and approximations. Section V is devoted to the influence of an electromagnetic dipole field on a conductor consisting of a few tight-binding levels. Situations with an ac transport voltage are addressed in Appendix A, while in Appendix B, we detail an alternative derivation which has been introduced in Ref. 30.

## II. LEAD-WIRE MODEL

We start out by introducing a model for the central conductor (“wire”) under the influence of an external driving field like, e.g., a molecular wire subject to laser radiation or coupled quantum dots<sup>1,3</sup> driven by microwaves or an oscillating gate voltage. The conductor is attached by tunneling couplings to external leads. The entire setup of our nanoscale system is described by the time-dependent Hamiltonian

$$H(t) = H_{\text{wire}}(t) + H_{\text{leads}} + H_{\text{contacts}}, \quad (1)$$

where the different terms correspond to the wire, the leads, and the wire-lead couplings, respectively. We focus on the regime of coherent quantum transport where the main physics at work occurs on the wire itself. In doing so, we neglect other possible influences originating from driving induced hot electrons in the leads, dissipation on the wire and, as well, electron-electron interaction effects. Then, the wire Hamiltonian reads in a tight-binding approximation with  $N$  orbitals  $|n\rangle$

$$H_{\text{wire}}(t) = \sum_{n,n'} H_{nn'}(t) c_n^\dagger c_{n'}. \quad (2)$$

For a molecular wire, this constitutes the so-called Hückel description where each site corresponds to one atom. The fermion operators  $c_n$ ,  $c_n^\dagger$  annihilate and create, respectively, an electron in the orbital  $|n\rangle$ . The influence of an applied ac field with frequency  $\Omega = 2\pi/T$  results in a periodic time-dependence of the wire Hamiltonian:  $H_{nn'}(t+T) = H_{nn'}(t)$ . The leads are modeled by ideal

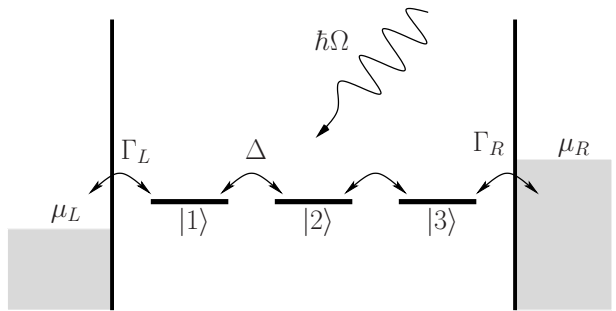


FIG. 1: Level structure of a nano-conductor with  $N = 3$  orbitals. The end sites are coupled to two leads with chemical potentials  $\mu_L$  and  $\mu_R = \mu_L + eV$ .

electron gases,

$$H_{\text{leads}} = \sum_q \epsilon_q (c_{Lq}^\dagger c_{Lq} + c_{Rq}^\dagger c_{Rq}), \quad (3)$$

where  $c_{Lq}^\dagger$  ( $c_{Rq}^\dagger$ ) creates an electron in the state  $|Lq\rangle$  ( $|Rq\rangle$ ) in the left (right) lead. The tunneling Hamiltonian

$$H_{\text{contacts}} = \sum_q \left( V_{Lq} c_{Lq}^\dagger c_1 + V_{Rq} c_{Rq}^\dagger c_N \right) + \text{h.c.} \quad (4)$$

establishes the contact between the sites  $|1\rangle$ ,  $|N\rangle$  and the respective lead, as sketched in Fig. 1. This tunneling coupling is described by the spectral density

$$\Gamma_\ell(\epsilon) = 2\pi \sum_q |V_{\ell q}|^2 \delta(\epsilon - \epsilon_q) \quad (5)$$

of lead  $\ell$ ,  $\ell = L, R$ . If the lead modes are dense,  $\Gamma_\ell(\epsilon)$  becomes a smooth function.

To fully specify the dynamics, we choose as an initial condition for the left/right lead a grand-canonical electron ensemble at temperature  $T$  and electro-chemical potential  $\mu_{L/R}$ , respectively. Thus, the initial density matrix reads

$$\rho_0 \propto e^{-(H_{\text{leads}} - \mu_L N_L - \mu_R N_R)/k_B T}, \quad (6)$$

where  $N_\ell = \sum_q c_{\ell q}^\dagger c_{\ell q}$  is the number of electrons in lead  $\ell$  and  $k_B T$  denotes the Boltzmann constant times temperature. An applied voltage  $V$  maps to a chemical potential difference  $\mu_R - \mu_L = eV$  with  $-e$  being the electron charge. Then, at initial time  $t_0$ , the only nontrivial expectation values of the wire operators read  $\langle c_{\ell'q'}^\dagger c_{\ell q} \rangle = f_\ell(\epsilon_q) \delta_{\ell\ell'} \delta_{qq'}$  where  $f_\ell(\epsilon) = (1 + \exp[(\epsilon - \mu_\ell)/k_B T])^{-1}$  denotes the Fermi function.

In our model Hamiltonian (1), the leads are time-independent. Thus, it seemingly cannot describe ac transport voltages. Such a situation, however, can be mapped by a gauge transformation to one with time-independent chemical potentials as demonstrated in Appendix A.

### III. SCATTERING APPROACH FOR TIME-DEPENDENT POTENTIALS

Due to their experimental accessibility, the central quantities in a quantum transport problem are the stationary current and the low-frequency part of its noise spectrum. Within a scattering picture of *non-driven* mesoscopic transport, both quantities can be expressed in terms of a transmission function  $T(E)$  which reflects the probability that an electron is transmitted from one lead to the other.<sup>33</sup> Due to energy conservation, the reversed process, occurs with equal probability. This is no longer true for driven systems and, consequently, the scattering approach needs to be generalized. Thus, in this section, we *derive* expressions for the currents and its noise properties for the transport through the time-dependent system modeled above. In the so-called wide-band limit, the more compact derivation presented in Ref. 30 becomes possible, cf. Appendix B. We will show that the average electrical current contains only transition probabilities and, thus, resembles a scattering formula. In clear contrast to the static two-terminal case, however, we will find that the noise depends in addition also on the phases of the scattering matrix.

#### A. Charge, current, and their fluctuations

To avoid the explicit appearance of commutators in the definition of correlation functions, we perform the derivation of the central transport quantities in the Heisenberg picture. As a starting point we choose the operator

$$Q_\ell(t) = eN_\ell(t) - eN_\ell(t_0) \quad (7)$$

that describes the charge accumulated in lead  $\ell$  with respect to the initial state. Due to total charge conservation,  $Q_\ell$  equals the net charge transmitted across the contact  $\ell$ ; its time derivative defines the corresponding current

$$I_\ell(t) = \frac{d}{dt}Q_\ell(t). \quad (8)$$

The current noise is described by the symmetrized correlation function

$$S_\ell(t, t') = \frac{1}{2} \langle [\Delta I_\ell(t), \Delta I_\ell(t')]_+ \rangle \quad (9)$$

of the current fluctuation operator  $\Delta I_\ell(t) = I_\ell(t) - \langle I_\ell(t) \rangle$ , where the anticommutator  $[A, B]_+ = AB + BA$  ensures hermiticity. It can be shown that at long times,  $S_\ell(t, t') = S_\ell(t + \mathcal{T}, t' + \mathcal{T})$  shares the time-periodicity of the driving.<sup>49</sup> Therefore, it is possible to characterize the noise level by the zero-frequency component of  $S_\ell(t, t - \tau)$  averaged over the driving period,

$$\bar{S}_\ell = \frac{1}{\mathcal{T}} \int_0^{\mathcal{T}} dt \int_{-\infty}^{\infty} d\tau S_\ell(t, t - \tau). \quad (10)$$

We find below that for two-terminal devices  $\bar{S}_\ell$  is independent of the contact  $\ell$ , i.e.,  $\bar{S}_L = \bar{S}_R \equiv \bar{S}$ .

The evaluation of the zero-frequency noise  $\bar{S}$  directly from its definition (10) can be tedious due to the explicit appearance of both times,  $t$  and  $t - \tau$ . This inconvenience can be circumvented by employing the relation

$$\frac{d}{dt} \left( \langle Q_\ell^2(t) \rangle - \langle Q_\ell(t) \rangle^2 \right) = 2 \int_0^\infty d\tau S_\ell(t, t - \tau) \quad (11)$$

which follows from the integral representation of Eqs. (7) and (8),  $Q_\ell(t) = \int_{t_0}^t dt' I_\ell(t')$ , in the limit  $t_0 \rightarrow -\infty$ . By averaging Eq. (11) over the driving period and using  $S(t, t - \tau) = S(t - \tau, t)$ , we obtain

$$\bar{S} = \left\langle \frac{d}{dt} \langle \Delta Q_\ell^2(t) \rangle \right\rangle_t, \quad (12)$$

where  $\Delta Q_\ell = Q_\ell - \langle Q_\ell \rangle$  denotes the charge fluctuation operator and  $\langle \dots \rangle_t$  the time average. The fact that the time average can be evaluated from the limit  $\bar{S} = \lim_{t_0 \rightarrow -\infty} \langle \Delta Q_\ell^2(t) \rangle / (t - t_0) > 0$  allows to interpret the zero-frequency noise as the “charge diffusion coefficient”. As a dimensionless measure for the *relative* noise strength, we employ the so-called Fano factor<sup>50,51</sup>

$$F = \frac{\bar{S}}{e|\bar{I}|}, \quad (13)$$

where  $\bar{I}$  denotes the time-average of the current expectation value  $\langle I_\ell(t) \rangle$ . Note that in a two-terminal device, the absolute value of the average current is independent of the contact  $\ell$ .

#### B. Transition amplitudes

In order to take the exclusion principle properly into account, we have formulated the transport problem under consideration in terms of second quantization. Nevertheless, in the absence of interactions, both the current and its noise can be traced back to the solution of the corresponding single-particle problem. Thus, our next step is to relate the expectation value and the variance of the charge operator (7) to the transmission of electrons from one lead to the other. For that purpose, we start from the Heisenberg equations of motion

$$\dot{c}_{L/Rq} = -\frac{i}{\hbar} \epsilon_q c_{L/Rq} - \frac{i}{\hbar} V_{L/Rq} c_{1/N}, \quad (14)$$

$$\dot{c}_{1/N} = -\frac{i}{\hbar} \sum_{n'} H_{1/N, n'}(t) c_{n'} - \frac{i}{\hbar} \sum_q V_{L/Rq}^* c_{L/Rq}, \quad (15)$$

$$\dot{c}_n = -\frac{i}{\hbar} \sum_{n'} H_{nn'}(t) c_{n'} \quad n = 2, \dots, N-1. \quad (16)$$

For these coupled linear equations, the formal solution

$$c_{\ell'q'}(t) = \sum_{\ell,q} \langle \ell'q' | U(t, t_0) | \ell q \rangle c_{\ell q}(t_0) + \sum_n \langle \ell'q' | U(t, t_0) | n \rangle c_n(t_0) \quad (17)$$

involves the propagator  $U(t, t_0)$  of the corresponding single-particle problem. We insert (17) into (7) and use the initial condition (6) to obtain for the transferred charge at long times [i.e., in the limit  $t_0 \rightarrow -\infty$ , where all transients die out and, in particular, the second line in Eq. (17) becomes irrelevant] the expectation value

$$\langle Q_L(t) \rangle = e \sum_{q',q,\ell} (|\langle Lq' | U(t, t_0) | \ell q \rangle|^2 - \delta_{\ell L} \delta_{qq'}) f_\ell(\epsilon_q). \quad (18)$$

To symmetrize this expression, we eliminate the back-scattering terms, i.e., the contributions with  $\ell = L$ , by employing the completeness relation

$$1 = \sum_q |Lq\rangle \langle Lq| + \sum_q |Rq\rangle \langle Rq| + \sum_n |n\rangle \langle n| \quad (19)$$

$$\equiv P_L + P_R + P_{\text{wire}}, \quad (20)$$

where  $P_L$ ,  $P_R$ , and  $P_{\text{wire}}$  denote the projectors onto the states of the left lead, the right lead, and the wire, respectively. Then, from the time derivative of Eq. (18), we find for the current through the left contact the result

$$\langle I_L(t) \rangle = e \sum_{q,q'} \{ w_{Lq',Rq}(t) f_R(\epsilon_q) - w_{Rq',Lq}(t) f_L(\epsilon_q) \} - e \sum_{n,q} w_{n,Lq}(t) f_L(\epsilon_q) \quad (21)$$

and *mutatis mutandis* for the current through the right contact. This expression already obeys the “scattering form” with the *time-dependent* transmission

$$T_{\ell'\ell}(t, \epsilon) = 2\pi\hbar \sum_{q,q'} w_{\ell'q',\ell q}(t) \delta(\epsilon - \epsilon_q) \quad (22)$$

of electrons with energy  $\epsilon$  from lead  $\ell$  to lead  $\ell'$ . At asymptotic times, the transitions from the lead state  $|\ell q\rangle$  to the lead state  $|\ell'q'\rangle$  and the wire state  $|n\rangle$  happen with the rates

$$w_{\ell'q',\ell q}(t) = \lim_{t_0 \rightarrow -\infty} \frac{d}{dt} |\langle \ell'q' | U(t, t_0) | \ell q \rangle|^2, \quad (23)$$

$$w_{n,\ell q}(t) = \lim_{t_0 \rightarrow -\infty} \frac{d}{dt} |\langle n | U(t, t_0) | \ell q \rangle|^2. \quad (24)$$

The last term in the current (21) describes a periodic charging of the wire stemming from the external driving. With an average over one driving period, this contribution vanishes and, thus, the dc current reads

$$\bar{I} = e \sum_{q,q'} \{ \bar{w}_{Lq',Rq} f_R(\epsilon_q) - \bar{w}_{Rq',Lq} f_L(\epsilon_q) \}, \quad (25)$$

with  $\bar{w}_{\ell'q',\ell q}$  denoting the time average of the rate (23). Interchanging in Eq. (25)  $L$  and  $R$  yields the negative current  $-\bar{I}$ . Thus, as expected from total charge conservation, the average current is, besides its sign, independent of the contact at which it is evaluated. We emphasize that (25) obeys the form of the current formula obtained for a *static* conductor within a scattering formalism. In particular, consistent with Refs. 32 and 38, no “Pauli blocking factors”  $(1 - f_\ell)$  appear in our derivation. In contrast to a static situation, this is in the present context relevant since for a driven system generally  $\bar{w}_{Lq,Rq'} \neq \bar{w}_{Rq',Lq}$ , such that a contribution proportional to  $f_L(\epsilon_{q'}) f_R(\epsilon_q)$  would not cancel.<sup>38,39</sup>

The zero-frequency noise  $\bar{S}$  is conveniently derived from the charge fluctuation with the help of relation (12). Expressing the charge fluctuation by the Heisenberg operators (17) yields for the initial condition (6) after some algebra

$$\begin{aligned} \langle \Delta Q_L^2(t) \rangle &= \sum_{q,q'} \{ f_R(\epsilon_{q'}) \bar{f}_R(\epsilon_q) |\langle Rq' | U^\dagger P_L U | Rq \rangle|^2 \\ &\quad + f_L(\epsilon_{q'}) \bar{f}_R(\epsilon_q) |\langle Lq' | U^\dagger P_L U | Rq \rangle|^2 \\ &\quad + f_L(\epsilon_{q'}) \bar{f}_L(\epsilon_q) |\langle Lq' | U^\dagger (P_R + P_{\text{wire}}) U | Lq \rangle|^2 \\ &\quad + f_R(\epsilon_{q'}) \bar{f}_L(\epsilon_q) |\langle Rq' | U^\dagger (P_R + P_{\text{wire}}) U | Lq \rangle|^2 \}. \end{aligned} \quad (26)$$

By using the completeness relation (19), we have achieved a form which is, besides the appearance of  $P_{\text{wire}}$ , symmetric under exchanging  $L \leftrightarrow R$ . Here,  $U$  is a shorthand notation for  $U(t, t_0)$  and  $\bar{f}_\ell = 1 - f_\ell$ . Taking the time derivative and averaging over the driving period yields

$$\begin{aligned} \bar{S} = e^2 \sum_{q,q'} \{ &W_{Rq',Rq}^L f_R(\epsilon_{q'}) \bar{f}_R(\epsilon_q) \\ &+ W_{Lq',Rq}^L f_L(\epsilon_{q'}) \bar{f}_R(\epsilon_q) \\ &+ W_{Lq',Lq}^R f_L(\epsilon_{q'}) \bar{f}_L(\epsilon_q) \\ &+ W_{Rq',Lq}^R f_R(\epsilon_{q'}) \bar{f}_L(\epsilon_q) \}, \end{aligned} \quad (27)$$

where we have defined

$$W_{\ell'q',\ell q}^{\ell''} = \lim_{t_0 \rightarrow -\infty} \left\langle \frac{d}{dt} |\langle \ell'q' | U^\dagger(t, t_0) P_{\ell''} U(t, t_0) | \ell q \rangle|^2 \right\rangle_t. \quad (28)$$

The contributions in Eq. (26) which contain the projector  $P_{\text{wire}}$  on the wire states do not contribute to the zero-frequency noise. This can be demonstrated by inserting for the propagator the explicit expressions (34) and (35) which we derive in the next subsection. Interestingly enough, the noise  $\bar{S}$  depends on both the diagonal and the off-diagonal elements of the projector  $U^\dagger P_{\ell''} U$ . By contrast, the current (21) depends only on the diagonal elements of this operator. As a consequence, in the presence of driving it is not possible to express the noise solely by transmission *probabilities*; cf. Eq. (45), below.

### C. Lead elimination

The evaluation of the rates  $w_{\ell'q',\ell q}$  and  $W_{\ell'q',\ell q}^{\ell''}$  involves the matrix elements of the time-evolution operator  $U(t, t_0)$  with the wire and the lead states. In the following, we eliminate the lead states and will find expressions for the rates that depend explicitly only on the propagator for the wire electrons and the spectral density of the couplings to the leads.

We start from the Schrödinger equation for the propagator,  $i\hbar\partial U(t, t')/\partial t = \mathcal{H}(t)U(t, t')$ , where  $\mathcal{H}(t)$  is the single-particle Hamiltonian underlying (1). Formal integration with the initial condition  $U(t', t') = \mathbf{1}$  results in the Dyson equation

$$U(t, t') = U_0(t, t') - \frac{i}{\hbar} \int_{t'}^t dt'' U_0(t, t'') \mathcal{H}_{\text{contacts}} U(t'', t'), \quad (29)$$

where  $U_0$  denotes the propagator in the absence of the wire-lead coupling. We emphasize that due to the explicit time-dependence of the wire Hamiltonian, the integral in (29) is not a mere convolution. Using  $\langle \ell'q' | U_0(t, t') | \ell q \rangle = \delta_{\ell\ell'} \delta_{qq'} \exp[-i\epsilon_q(t - t')/\hbar]$ , we find for the transition matrix elements the relations

$$\langle n | U(t, t_0) | \ell q \rangle = -\frac{i}{\hbar} V_{\ell q}^* \int_{t_0}^t dt' e^{-\frac{i}{\hbar}\epsilon_q(t' - t_0)} \langle n | U(t, t') | n_\ell \rangle \quad (30)$$

and

$$\begin{aligned} \langle \ell'q' | U(t, t_0) | \ell q \rangle &= e^{-\frac{i}{\hbar}(\epsilon_{q'}t - \epsilon_q t_0)} \left\{ \delta_{\ell\ell'} \delta_{qq'} - \frac{V_{\ell'q'} V_{\ell q}^*}{\hbar^2} \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' \right. \\ &\quad \left. \times e^{\frac{i}{\hbar}(\epsilon_{q'}t' - \epsilon_q t'')} \langle n_{\ell'} | U(t', t'') | n_\ell \rangle \right\}, \quad (31) \end{aligned}$$

where  $n_\ell$  denotes the wire site attached to lead  $\ell$ , i.e.,  $n_L = 1$  and  $n_R = N$ .

At this stage, it is convenient to make use of the time-periodicity of the Hamiltonian,  $\mathcal{H}(t) = \mathcal{H}(t + \mathcal{T})$ . This

has the consequence<sup>52</sup> that  $U(t, t') = U(t + \mathcal{T}, t' + \mathcal{T})$  and, thus, the retarded Green function

$$G(t, \epsilon) = -\frac{i}{\hbar} \int_0^\infty d\tau e^{\frac{i}{\hbar}\epsilon\tau} U(t, t - \tau) = G(t + \mathcal{T}, \epsilon) \quad (32)$$

can be decomposed into a Fourier series,  $G(t, \epsilon) = \sum_{k=-\infty}^\infty e^{-ik\Omega t} G^{(k)}(\epsilon)$ , with the coefficients

$$G^{(k)}(\epsilon) = \frac{1}{\mathcal{T}} \int_0^\mathcal{T} dt e^{ik\Omega t} G(t, \epsilon). \quad (33)$$

Physically,  $G^{(k)}(\epsilon)$  describes the propagation of an electron with initial energy  $\epsilon$  under the absorption (emission) of  $|k|$  photons for  $k > 0$  ( $k < 0$ ). We emphasize that generally all sidebands  $k = -\infty \dots \infty$  contribute to the Green function (32) and that, consequently, the  $k$ -summations are unrestricted.

After making use of Eqs. (32) and (33), the transition amplitudes (30) and (31) become

$$\langle n | U(t, t_0) | \ell q \rangle = V_{\ell q}^* e^{-\frac{i}{\hbar}\epsilon_q(t - t_0)} \sum_k e^{-ik\Omega t} \langle n | G^{(k)}(\epsilon_q) | n_\ell \rangle \quad (34)$$

and

$$\begin{aligned} \langle \ell'q' | U(t, t_0) | \ell q \rangle &= e^{-\frac{i}{\hbar}(\epsilon_{q'}t - \epsilon_q t_0)} \left\{ \delta_{\ell\ell'} \delta_{qq'} - \sum_k V_{\ell'q'} V_{\ell q}^* \right. \\ &\quad \left. \times \frac{e^{\frac{i}{\hbar}(\epsilon_{q'} - \epsilon_q - k\hbar\Omega - i\eta)t}}{\epsilon_{q'} - \epsilon_q - k\hbar\Omega - i\eta} \langle n_{\ell'} | G^{(k)}(\epsilon_q) | n_\ell \rangle \right\}, \quad (35) \end{aligned}$$

respectively. Since below we restrict ourselves to asymptotic times,  $t_0 \rightarrow -\infty$ , we have shifted the lower limit of the integrals accordingly. Moreover, in order to perform the  $t'$ -integration in Eq. (31), we have introduced a converging factor  $e^{\eta t'}/\hbar$  and will finally consider the limit  $\eta \rightarrow 0$ .

#### 1. Average current

For the further evaluation of the average current (25), we insert the transition amplitude (35) into (23). After taking the time derivative, averaging over time  $t$ , and considering the limit  $\eta \rightarrow 0$ , we find

$$\bar{w}_{Lq',Rq} = \frac{2\pi}{\hbar} |V_{Lq'} V_{Rq}|^2 \sum_k |G_{1N}^{(k)}(\epsilon_q)|^2 \delta(\epsilon_{q'} - \epsilon_q - k\hbar\Omega), \quad (36)$$

and the corresponding expression for  $\bar{w}_{Rq',Lq}$ . We have introduced the notation  $G_{nn'} = \langle n | G | n' \rangle$ . By use of the spectral density (5), we replace the remaining sums over the lead states by energy integrals and obtain as our first main result the dc current

$$\bar{I} = \frac{e}{\hbar} \sum_{k=-\infty}^\infty \int d\epsilon \left\{ T_{LR}^{(k)}(\epsilon) f_R(\epsilon) - T_{RL}^{(k)}(\epsilon) f_L(\epsilon) \right\}, \quad (37)$$

where

$$T_{LR}^{(k)}(\epsilon) = \Gamma_L(\epsilon + k\hbar\Omega)\Gamma_R(\epsilon)|G_{1N}^{(k)}(\epsilon)|^2, \quad (38)$$

$$T_{RL}^{(k)}(\epsilon) = \Gamma_R(\epsilon + k\hbar\Omega)\Gamma_L(\epsilon)|G_{N1}^{(k)}(\epsilon)|^2, \quad (39)$$

denote the transmission probabilities for electrons from the right lead, respectively from the left lead, with initial energy  $\epsilon$  and final energy  $\epsilon + k\hbar\Omega$ , i.e., the probability for an scattering event under the absorption (emission) of  $|k|$  photons if  $k > 0$  ( $k < 0$ ).

For a static situation, the transmissions  $T_{LR}^{(k)}(\epsilon)$  and  $T_{RL}^{(k)}(\epsilon)$  are identical and contributions with  $k \neq 0$  vanish. Thus, it is possible to write the current (37) as a product of a *single* transmission  $T(\epsilon)$  and the difference of the Fermi functions,  $f_R(\epsilon) - f_L(\epsilon)$ . We emphasize that in the driven case this is no longer true.

## 2. ac current

Although below we focus on the computation of dc currents, we here continue the derivation of the transport quantities by presenting explicit expressions for the ac currents. We restrict ourselves to  $\langle I_L(t) \rangle$  since  $\langle I_R(t) \rangle$  simply follows by proper index replacements. Evaluating  $\langle I_L(t) \rangle$ , we consider also the last term in Eq. (21) which describes a periodic charging/discharging of the wire. Apart from the time average we perform the same steps as in the derivation of the dc current and obtain

$$\langle I_L(t) \rangle = \frac{e}{h} \int d\epsilon \{ T_{LR}(t, \epsilon) f_R(\epsilon) - T_{RL}(t, \epsilon) f_L(\epsilon) \} - \dot{q}_L(t) \quad (40)$$

where

$$q_L(t) = \frac{e}{2\pi} \int d\epsilon \Gamma_L(\epsilon) \sum_n \left| \sum_k e^{-ik\Omega t} G_{n1}^{(k)}(\epsilon) \right|^2 f_L(\epsilon) \quad (41)$$

denotes the charge oscillating between the left lead and the wire. Obviously, since  $q_L(t)$  is time-periodic and bounded, its time derivative cannot contribute to the average current. The corresponding charge arising from the right lead,  $q_R(t)$ , is *a priori* unrelated to  $q_L(t)$ ; the actual charge on the wire reads  $q_L(t) + q_R(t)$ . The time-dependent current is determined by the time-dependent transmission

$$T_{LR}(t, \epsilon) = \Gamma_R(\epsilon) \operatorname{Re} \sum_{k, k'} e^{-ik\Omega t} G_{1N}^{(k'+k)}(\epsilon) [G_{1N}^{(k')}(\epsilon)]^* \left[ \Gamma_L(\epsilon + k'\hbar\Omega) + \frac{i}{\pi} \mathcal{P} \int d\epsilon' \frac{\Gamma_L(\epsilon')}{\epsilon' - \epsilon - k'\hbar\Omega} \right]. \quad (42)$$

The corresponding expression for  $T_{RL}(t, \epsilon)$  follows from the replacement  $(L, 1) \leftrightarrow (R, N)$ . Note that in the wide-band limit  $\Gamma_\ell(\epsilon) = \Gamma_\ell$ ,  $\ell = L, R$ , the contribution from the principal value integral vanishes.

## 3. zero-frequency noise

In order to obtain the zero-frequency noise  $\bar{S}$ , we evaluate the rates  $W_{\ell'q', \ell q}^{\ell''}$ . This step is performed along the lines of reasoning for the evaluation of  $\bar{w}_{\ell'q', \ell q}$  (although the actual calculation is far more tedious): We insert the transition amplitude (35) into (28), take the derivative with respect to  $t$ , and average over one driving period. Finally, we employ the relation  $\lim_{\eta \rightarrow 0} 4\eta[(\epsilon - a - i\eta)(\epsilon - b + i\eta)(\epsilon' - b - i\eta)(\epsilon' - a + i\eta)]^{-1} = (2\pi)^3 \delta(\epsilon - a) \delta(\epsilon' - b) \delta(a - b)$  to perform the limit  $\eta \rightarrow 0$  and find

$$W_{Rq', Rq}^L = \frac{2\pi}{h} |V_{Rq'}|^2 |V_{Rq}|^2 \sum_k \left| \sum_{k'} \Gamma_L(\epsilon_q + k'\hbar\Omega) [G_{1N}^{(k'-k)}(\epsilon_{q'})]^* G_{1N}^{(k')}(\epsilon_q) \right|^2 \delta(\epsilon_{q'} - \epsilon_q - k\hbar\Omega), \quad (43)$$

$$W_{Lq', Rq}^L = \frac{2\pi}{h} |V_{Lq'}|^2 |V_{Rq}|^2 \sum_k \left| \sum_{k'} \Gamma_L(\epsilon_q + k'\hbar\Omega) [G_{11}^{(k'-k)}(\epsilon_{q'})]^* G_{1N}^{(k')}(\epsilon_q) - i G_{1N}^{(k)}(\epsilon_q) \right|^2 \delta(\epsilon_{q'} - \epsilon_q - k\hbar\Omega). \quad (44)$$

The corresponding expressions for  $W_{Lq',Lq}^R$  and  $W_{Rq',Lq}^R$  follow from the replacement  $(L, 1) \leftrightarrow (R, N)$ . Inserting these into the noise expression (27) we arrive at our central result

$$\begin{aligned} \bar{S} = \frac{e^2}{h} \sum_k \int d\epsilon \left\{ \Gamma_R(\epsilon_k) \Gamma_R(\epsilon) \left| \sum_{k'} \Gamma_L(\epsilon_{k'}) G_{1N}^{(k'-k)}(\epsilon_k) [G_{1N}^{(k')}(\epsilon)]^* \right|^2 f_R(\epsilon) \bar{f}_R(\epsilon_k) \right. \\ \left. + \Gamma_R(\epsilon_k) \Gamma_L(\epsilon) \left| \sum_{k'} \Gamma_L(\epsilon_{k'}) G_{1N}^{(k'-k)}(\epsilon_k) [G_{11}^{(k')}(\epsilon)]^* - i G_{1N}^{(-k)}(\epsilon_k) \right|^2 f_L(\epsilon) \bar{f}_R(\epsilon_k) \right\} \\ + \text{same terms with the replacement } (L, 1) \leftrightarrow (R, N). \end{aligned} \quad (45)$$

We have defined  $\epsilon_k = \epsilon + k\hbar\Omega$  and replaced the sums over the lead states by energy integrations using the spectral density (5).

#### D. Wide-band limit and Floquet theory

In order to evaluate the expressions for  $\bar{I}$  and  $\bar{S}$  further, we derive an eigenfunction representation for the Green function. It is well-known that beyond the adiabatic limit, the eigenfunctions of the Hamiltonian are not of particular use — rather a proper basis is provided by a Floquet ansatz.<sup>52,53,54</sup>

Let us start from the Schrödinger equation for the propagator,

$$i\hbar \frac{d}{dt} \langle n|U(t, t_0)|n' \rangle = \sum_{n''} H_{nn''}(t) \langle n''|U(t, t_0)|n' \rangle, \quad (46)$$

for  $n = 2, \dots, N-1$ , and

$$\begin{aligned} i\hbar \frac{d}{dt} \langle n_\ell|U(t, t_0)|n' \rangle = \sum_{n''} H_{n_\ell n''}(t) \langle n''|U(t, t_0)|n' \rangle \\ + \sum_q V_{\ell q}^* \langle \ell q|U(t, t_0)|n' \rangle, \end{aligned} \quad (47)$$

where  $n_\ell$  is defined by  $n_L = 1$  and  $n_R = N$ . To eliminate the lead states in the second line of Eq. (47), we insert (30) and replace by use of the spectral density (5) the sum over the lead states by an energy integral. Then the last term in Eq. (47) becomes

$$-\frac{i}{2\pi\hbar} \int d\epsilon \Gamma_\ell(\epsilon) \int_{t_0}^t dt' e^{-i\epsilon(t'-t_0)/\hbar} \langle n_\ell|U(t, t')|n' \rangle. \quad (48)$$

Within the present context, we are mainly interested in the influence of the driving field on the conductor and not in the details of the coupling to the leads. Therefore, we choose for  $\Gamma_\ell(\epsilon)$  a rather generic form by assuming that in the relevant regime, it is practically energy-independent,

$$\Gamma_\ell(\epsilon) \longrightarrow \Gamma_\ell. \quad (49)$$

This so-called wide-band limit allows further progress since we now can perform in Eq. (48) the remaining energy integration to obtain  $\hbar\delta(t' - t_0)$  and, consequently,

Eq. (47) becomes

$$\begin{aligned} i\hbar \frac{d}{dt} \langle n_\ell|U(t, t_0)|n' \rangle = \sum_{n''} H_{n_\ell n''}(t) \langle n''|U(t, t_0)|n' \rangle \\ - \frac{i}{2} \Gamma_\ell \langle n_\ell|U(t, t_0)|n' \rangle. \end{aligned} \quad (50)$$

Equations (46) and (50), together with the initial conditions  $\langle n|U(t, t)|n' \rangle = \delta_{nn'}$  fully determine the propagator. Solving this linear set of equations is equivalent to computing a complete set of solutions for the equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = (\mathcal{H}_{\text{wire}}(t) - i\Sigma) |\psi(t)\rangle, \quad (51)$$

where the self-energy

$$\Sigma = |1\rangle \frac{\Gamma_L}{2} \langle 1| + |N\rangle \frac{\Gamma_R}{2} \langle N| \quad (52)$$

results from the coupling to the leads.

Equation (51) is linear and possesses time-dependent,  $\mathcal{T}$ -periodic coefficients. Thus, it is possible to construct a complete solution with the Floquet ansatz

$$|\psi_\alpha(t)\rangle = \exp[(-i\epsilon_\alpha/\hbar - \gamma_\alpha)t] |u_\alpha(t)\rangle, \quad (53)$$

$$|u_\alpha(t)\rangle = \sum_{k=-\infty}^{\infty} |u_{\alpha,k}\rangle \exp(-ik\Omega t). \quad (54)$$

The so-called Floquet states  $|u_\alpha(t)\rangle$  obey the time-periodicity of  $\mathcal{H}_{\text{wire}}(t)$  and have been decomposed into a Fourier series. In a Hilbert space that is extended by a periodic time coordinate, the so-called Sambe space,<sup>54</sup> they obey the Floquet eigenvalue equation<sup>52,55</sup>

$$\left( \mathcal{H}_{\text{wire}}(t) - i\Sigma - i\hbar \frac{d}{dt} \right) |u_\alpha(t)\rangle = (\epsilon_\alpha - i\hbar\gamma_\alpha) |u_\alpha(t)\rangle. \quad (55)$$

Due to the Brillouin zone structure of the Floquet spectrum,<sup>52,53,54</sup> it is sufficient to compute all eigenvalues of the first Brillouin zone,  $-\hbar\Omega/2 < \epsilon_\alpha \leq \hbar\Omega/2$ . Since the operator on the l.h.s. of Eq. (55) is non-Hermitian, the eigenvalues  $\epsilon_\alpha - i\hbar\gamma_\alpha$  are generally complex valued and the (right) eigenvectors are not mutually orthogonal. Thus, to determine the propagator, we need to

solve also the adjoint Floquet equation yielding again the same eigenvalues but providing the adjoint eigenvectors  $|u_\alpha^+(t)\rangle$ . It can be shown that the Floquet states  $|u_\alpha(t)\rangle$  together with the adjoint states  $|u_\alpha^+(t)\rangle$  form at equal times a complete bi-orthogonal basis:  $\langle u_\alpha^+(t)|u_\beta(t)\rangle = \delta_{\alpha\beta}$  and  $\sum_\alpha |u_\alpha(t)\rangle\langle u_\alpha^+(t)| = \mathbf{1}$ . A proof requires to account for the time-periodicity of the Floquet states since the eigenvalue equation (55) holds in a Hilbert space extended by a periodic time coordinate.<sup>52,56</sup>

Using the Floquet equation (55), it is straightforward to show that with the help of the Floquet states  $|u_\alpha(t)\rangle$  the propagator can be written as

$$U(t, t') = \sum_\alpha e^{-i(\epsilon_\alpha/\hbar - i\gamma_\alpha)(t-t')} |u_\alpha(t)\rangle\langle u_\alpha^+(t')|, \quad (56)$$

where the sum runs over all Floquet states within one Brillouin zone. Consequently, the Fourier coefficients of the Green function [cf. Eq. (33)] read

$$G^{(k)}(\epsilon) = -\frac{i}{\hbar} \int_0^T \frac{dt}{T} e^{ik\Omega t} \int_0^\infty d\tau e^{i\epsilon\tau/\hbar} U(t, t-\tau) \quad (57)$$

$$= \sum_\alpha \sum_{k'=-\infty}^\infty \frac{|u_{\alpha, k'+k}\rangle\langle u_{\alpha, k'}^+|}{\epsilon - (\epsilon_\alpha + k'\hbar\Omega - i\hbar\gamma_\alpha)}. \quad (58)$$

Inserting them into Eqs. (37) and (45) yields explicit expressions for the current and the noise, respectively.

#### IV. LIMITING CASES

In the previous section, the dc current and the zero-frequency noise have been derived for a periodic but otherwise arbitrary driving. Within the wide-band limit, both quantities can be expressed in terms of the solutions of the Floquet equation (55), i.e., the solution of a non-Hermitian eigenvalue problem in an extended Hilbert space. Thus, for large systems, the numerical computation of the Floquet states can be rather costly. Moreover, for finite temperatures, the energy integration in the expressions (37) and (45) has to be performed numerically. Therefore, approximation schemes which allow a more efficient computation are of much practical use.

Before introducing various approximation schemes for the wire propagator, we discuss two particular cases for which current and noise assume more intuitive expressions. In doing so, we define quantities to which we will refer later in this section.

##### A. Static conductor and adiabatic limit

For consistency, the expressions (37) and (45) for the dc current and the zero-frequency noise, respectively, must coincide in the undriven limit with the corresponding expressions of the time-independent scattering theory.<sup>33</sup> This is indeed the case since the static situation is characterized by two relations: First, in the absence of

spin-dependent interactions, we have time-reversal symmetry,  $w_{Lq', Rq} = w_{Rq, Lq'}$  and, second, all sidebands with  $k \neq 0$  vanish, i.e.,  $T_{RL}^{(k)}(\epsilon) = T_{LR}^{(k)}(\epsilon) = \delta_{k,0}T(\epsilon)$ , where

$$T(\epsilon) = \Gamma_L(\epsilon)\Gamma_R(\epsilon)|G_{1N}(\epsilon)|^2 \quad (59)$$

and  $G(\epsilon)$  is the Green function in the undriven limit. Then the current assumes the known form

$$I_0 = \frac{e}{h} \int d\epsilon T(\epsilon) [f_R(\epsilon) - f_L(\epsilon)]. \quad (60)$$

Moreover in a static situation, the relation<sup>32,57</sup>

$$|\Gamma_L(\epsilon)G_{11}(\epsilon) + i|^2 = 1 - T(\epsilon), \quad (61)$$

allows to eliminate the backscattering terms in the second line of Eq. (45) such that the zero-frequency noise can be expressed solely in terms of the transmission to read<sup>33</sup>

$$S_0 = \frac{e^2}{h} \int d\epsilon \left\{ T(\epsilon) [f_L(\epsilon)\bar{f}_L(\epsilon) + f_R(\epsilon)\bar{f}_R(\epsilon)] + T(\epsilon) [1 - T(\epsilon)] [f_R(\epsilon) - f_L(\epsilon)]^2 \right\}. \quad (62)$$

For zero temperature, the terms in the first line vanish and pure shot noise remains. In contrast, for zero voltage,  $f_R = f_L$  and the terms in the first line constitute equilibrium quantum noise. Obviously if both voltage and temperature are zero, not only the current but also the noise vanishes. In the presence of driving, this is no longer the case. This becomes particularly evident in the high-frequency limit studied in Sec. IV E.

It is known that in the adiabatic limit, i.e., for small driving frequencies, the numerical solution of the Floquet equation (55) becomes infeasible because a diverging number of sidebands has to be taken into account. In more mathematical terms, Floquet theory has no proper limit as  $\Omega \rightarrow 0$ .<sup>58</sup> The practical consequence of this is that for low driving frequencies, it is favorable to tackle the transport problem with a different strategy: If  $\hbar\Omega$  is the smallest energy-scale of the Hamiltonian (1), one computes for the “frozen” Hamiltonian at each instance of time the current and the noise from the static expressions (60) and (62) being followed up by time-averaging.

##### B. Infinite voltage

Many phenomena can be discussed in the limit of very large (practically infinite; subscript  $\infty$ ) voltages such that  $f_R \rightarrow 1$  and  $f_L \rightarrow 0$  in the relevant energy range. Then, the dc current (37) becomes

$$\bar{I}_\infty = \frac{e}{h} \sum_k \int d\epsilon \Gamma_L(\epsilon + k\hbar\Omega)\Gamma_R(\epsilon)|G_{1N}^{(k)}(\epsilon)|^2. \quad (63)$$

In the zero-frequency noise (45), only the contribution with  $f_R\bar{f}_L$  remains, thus,  $\bar{S}_\infty = e^2 \sum_{q', q} W_{Rq', Lq}^R =$



$e^2 \sum_{q,q'} (w_{Rq',Lq} - W_{Lq',Lq}^R)$ . To derive this expression, we again have used the completeness relation (19) and the fact that terms containing the projector on the wire states do not contribute to time averages. Expressing  $w_{Rq',Lq}$  and  $W_{Lq',Lq}^R$  by the Green functions yields

$$\bar{S}_\infty = e\bar{I}_\infty - \frac{e^2}{\hbar} \sum_k \int d\epsilon \Gamma_L(\epsilon_k) \Gamma_L(\epsilon) \times \left| \sum_{k'} \Gamma_R(\epsilon_{k'}) G_{N1}^{(k'-k)}(\epsilon_k) [G_{N1}^{(k')}(\epsilon)]^* \right|^2, \quad (64)$$

where  $\epsilon_k = \epsilon + k\hbar\Omega$ . These expressions make explicit that  $\bar{I}_\infty > 0$  and  $\bar{S}_\infty < e\bar{I}_\infty$ . Consequently, for infinite voltage the Fano factor (13) cannot exceed unity.

### C. Weak wire-lead coupling

In the limit of a weak wire-lead coupling, i.e., for coupling constants  $\Gamma_\ell$  which are far lower than all other energy scales of the wire Hamiltonian, it is possible to derive within a master equation approach a closed expression for the dc current.<sup>59</sup> The corresponding approximation within the present Floquet approach is based on treating the self-energy contribution  $-i\Sigma$  in the non-Hermitian Floquet equation (55) as a perturbation. Then, the zeroth order of the Floquet equation

$$\left( \mathcal{H}_{\text{wire}}(t) - i\hbar \frac{d}{dt} \right) |\phi_\alpha(t)\rangle = \epsilon_\alpha^0 |\phi_\alpha(t)\rangle, \quad (65)$$

describes the driven wire in the absence of the leads, where  $|\phi_\alpha(t)\rangle = \sum_k \exp(-ik\Omega t) |\phi_{\alpha,k}\rangle$  are the “usual” Floquet states with quasienergies  $\epsilon_\alpha^0$ . In the absence of degeneracies the first order correction to the quasienergies is  $-i\hbar\gamma_\alpha^1$  where

$$\gamma_\alpha^1 = \frac{1}{\hbar} \int_0^T \frac{dt}{T} \langle \phi_\alpha(t) | \Sigma | \phi_\alpha(t) \rangle \quad (66)$$

$$= \frac{\Gamma_L}{2\hbar} \sum_k |\langle 1 | \phi_{\alpha,k} \rangle|^2 + \frac{\Gamma_R}{2\hbar} \sum_k |\langle N | \phi_{\alpha,k} \rangle|^2. \quad (67)$$

Since the first-order correction to the Floquet states will contribute to neither the current nor the noise, the zeroth-order contribution  $|u_\alpha(t)\rangle = |u_\alpha^+(t)\rangle = |\phi_\alpha(t)\rangle$  is already sufficient for the present purpose. Consequently, the transmission (38) assumes the form

$$T_{LR}^{(k)}(\epsilon) = \Gamma_L \Gamma_R \sum_{\alpha,\beta,k',k''} \frac{\langle N | \phi_{\alpha,k'} \rangle \langle \phi_{\alpha,k'+k} | 1 \rangle}{\epsilon - (\epsilon_\alpha^0 + k'\hbar\Omega + i\hbar\gamma_\alpha^1)} \times \frac{\langle 1 | \phi_{\beta,k''+k} \rangle \langle \phi_{\beta,k''} | N \rangle}{\epsilon - (\epsilon_\beta^0 + k''\hbar\Omega - i\hbar\gamma_\beta^1)} \quad (68)$$

and  $T_{RL}^{(k)}(\epsilon)$  accordingly. The transmission (68) exhibits for small values of  $\Gamma_\ell$  sharp peaks at energies  $\epsilon_\alpha^0 + k'\hbar\Omega$  and  $\epsilon_\beta^0 + k''\hbar\Omega$  with widths  $\hbar\gamma_\alpha^1$  and  $\hbar\gamma_\beta^1$ . Therefore,

the relevant contributions to the sum come from terms for which the peaks of both factors coincide and, in the absence of degeneracies in the quasienergy spectrum, we keep only terms with

$$\alpha = \beta, \quad k' = k''. \quad (69)$$

Then, the fraction in (68) is a Lorentzian and can be approximated by  $\pi\delta(\epsilon - \epsilon_\alpha^0 - k'\hbar\Omega)/\hbar\gamma_\alpha^1$  provided that  $\gamma_\alpha^1$  is small. Consequently, the energy integration in (37) can be performed even for finite temperature and we obtain for the dc current the expression

$$\bar{I} = \frac{e}{\hbar} \sum_{\alpha,k,k'} \frac{\Gamma_{L\alpha k} \Gamma_{R\alpha k'}}{\Gamma_{L\alpha} + \Gamma_{R\alpha}} [f_R(\epsilon_\alpha^0 + k'\hbar\Omega) - f_L(\epsilon_\alpha^0 + k\hbar\Omega)]. \quad (70)$$

The coefficients

$$\Gamma_{L\alpha k} = \Gamma_L |\langle 1 | \phi_{\alpha,k} \rangle|^2, \quad \Gamma_{L\alpha} = \sum_k \Gamma_{L\alpha k}, \quad (71)$$

$$\Gamma_{R\alpha k} = \Gamma_R |\langle N | \phi_{\alpha,k} \rangle|^2, \quad \Gamma_{R\alpha} = \sum_k \Gamma_{R\alpha k}, \quad (72)$$

denote the overlap of the  $k$ th sideband  $|\phi_{\alpha,k}\rangle$  of the Floquet state  $|\phi_\alpha(t)\rangle$  with the first site and the last site of the wire, respectively. We have used  $2\hbar\gamma_\alpha^1 = \Gamma_{L\alpha} + \Gamma_{R\alpha}$  which follows from (67). Expression (70) has been derived in a prior work<sup>59</sup> within a rotating-wave approximation of a Floquet master equation approach.

Within the same approximation, we expand the zero-frequency noise (45) to lowest order in  $\Gamma_\ell$ : After inserting the spectral representation (58) of the Green function, we again keep only terms with identical Floquet index  $\alpha$  and identical sideband index  $k$  to obtain

$$\bar{S} = \frac{e^2}{\hbar} \sum_{\alpha,k,k'} \frac{\Gamma_{R\alpha k} \bar{f}_R(\epsilon_\alpha^0 + k'\hbar\Omega)}{(\Gamma_{L\alpha} + \Gamma_{R\alpha})^3} \{ 2\Gamma_{L\alpha}^2 \Gamma_{R\alpha k} f_R(\epsilon_\alpha^0 + k\hbar\Omega) + (\Gamma_{L\alpha}^2 + \Gamma_{R\alpha}^2) \Gamma_{L\alpha k} f_L(\epsilon_\alpha^0 + k\hbar\Omega) \} + \text{same terms with the replacement } L \leftrightarrow R. \quad (73)$$

Of particular interest for the comparison to the static situation is the limit of a large applied voltage such that practically  $f_R = 1$  and  $f_L = 0$ . Then, in Eqs. (70) and (73), the sums over the sideband indices  $k$  can be carried out such that

$$\bar{I}_\infty = \frac{e}{\hbar} \sum_\alpha \frac{\Gamma_{L\alpha} \Gamma_{R\alpha}}{\Gamma_{L\alpha} + \Gamma_{R\alpha}}, \quad (74)$$

$$\bar{S}_\infty = \frac{e^2}{\hbar} \sum_\alpha \frac{\Gamma_{L\alpha} \Gamma_{R\alpha} (\Gamma_{L\alpha}^2 + \Gamma_{R\alpha}^2)}{(\Gamma_{L\alpha} + \Gamma_{R\alpha})^3}. \quad (75)$$

These expressions resemble the corresponding expressions for the transport across a *static* double barrier.<sup>33</sup> If now  $\Gamma_{L\alpha} = \Gamma_{R\alpha}$  for all Floquet states  $|\phi_\alpha(t)\rangle$ , we find  $F = 1/2$ . This is in particular the case for systems obeying reflection symmetry.<sup>60</sup> In the presence of such symmetries, however, the existence of exact crossings, i.e. degeneracies, limits the applicability of the weak-coupling approximation.

### D. Homogeneous ac driving

In many experimental situations, the driving field acts as a time-dependent gate voltage, i.e., it merely shifts all on-site energies of the wire uniformly. Thus, the wire Hamiltonian is of the form

$$\mathcal{H}_{\text{wire}}(t) = \mathcal{H}_0 + f(t) \sum_n |n\rangle\langle n|, \quad (76)$$

where, without loss of generality, we restrict  $f(t)$  to possess zero time-average. A particular case of such a homogeneous driving is realized with a system that consists of only one level.<sup>42,61,62</sup> Then trivially, the time and the position dependence of the Floquet states factorize and, therefore, the dc current can be obtained within the formalism introduced by Tien and Gordon.<sup>8</sup> Here, we establish the relation between such a treatment and the present Floquet approach.

Since the time-dependent part of the Hamiltonian is proportional to the unity operator, the solution of the Floquet equation (55) is, besides a phase factor, given by the eigenfunctions  $|\alpha\rangle$  of the static operator  $\mathcal{H}_0 - i\Sigma$ ,

$$|u_\alpha(t)\rangle = e^{-iF(t)}|\alpha\rangle, \quad (77)$$

where  $(\mathcal{H}_0 - i\Sigma)|\alpha\rangle = (\epsilon_\alpha - i\hbar\gamma_\alpha)|\alpha\rangle$  and  $dF(t)/dt = f(t)/\hbar$ . The quasienergies  $(\epsilon_\alpha - i\hbar\gamma_\alpha)$  coincide with the eigenvalues of the static eigenvalue problem. Note that  $F(t)$  obeys the  $\mathcal{T}$ -periodicity of the driving field since the

time-average of  $f(t)$  vanishes by definition. Thus, the phase factor in the Floquet states (77) can be written as a Fourier series,

$$e^{-iF(t)} = \sum_k a_k e^{-ik\Omega t} \quad (78)$$

and, consequently we find  $|u_{\alpha,k}\rangle = a_k|\alpha\rangle$  and the adjoint states accordingly. Then, the Green function (33) becomes

$$G^{(k)}(\epsilon) = \sum_{k'} a_{k'+k} a_{k'}^* G(\epsilon - k'\hbar\Omega), \quad (79)$$

where  $G(\epsilon)$  denotes the Green function in the absence of the driving field. Inserting (79) into (37) and employing the sum rule  $\sum_{k'} a_{k'}^* a_{k'+k} = \delta_{k,0}$ , yields

$$\bar{I} = \sum_k |a_k|^2 \frac{e}{\hbar} \int d\epsilon T(\epsilon - k\hbar\Omega) [f_R(\epsilon) - f_L(\epsilon)], \quad (80)$$

where  $T(\epsilon)$  is the transmission in the absence of the driving. This expression allows the interpretation, that for homogeneous driving, the Floquet channels contribute *independently* to the current  $\bar{I}$ . For the special case of a one-site conductor and a sinusoidal driving, this relation to the static situation has been discussed in Refs. 61 and 62.

Addressing the noise properties, we obtain by inserting the Green function (79) into (45) the expression

$$\begin{aligned} \bar{S} = & \frac{e^2}{\hbar} \sum_k \int d\epsilon \left\{ \left| \sum_{k'} a_{k'+k}^* a_{k'} T(\epsilon - k'\hbar\Omega) \right|^2 f_R(\epsilon) \bar{f}_R(\epsilon + k\hbar\Omega) \right. \\ & + \Gamma_L \Gamma_R \left| \sum_{k'} a_{k'+k}^* a_{k'} G_{1N}(\epsilon - k'\hbar\Omega) [\Gamma_L G_{11}^*(\epsilon - k'\hbar\Omega) - i] \right|^2 f_L(\epsilon) \bar{f}_R(\epsilon + k\hbar\Omega) \\ & \left. + \text{same terms with the replacement } (L, 1) \leftrightarrow (R, N) \right\}. \end{aligned} \quad (81)$$

While the term in the first line contains only the static transmission at energies shifted by multiples of the photon energies, the contribution in the second line cannot be brought into such a convenient form. The reason for this is that the sum over  $k'$  inhibits the application of the relation (61). As a consequence, in clear contrast to the dc current, the zero-frequency noise cannot be interpreted in terms of independent Floquet channels. Only in the limit of large driving frequencies, we find below that the channels become effectively independent and (81) reduces to an expression that depends only on the transmission in the absence of the driving and the Fourier coefficients  $a_k$ , cf. next subsection.

Expressions for the dc current and the noise that depend only on the static transmission have been de-

rived by Tucker and Feldman<sup>63,64</sup> within a Tien-Gordon approach.<sup>8</sup> The central approximation of this approach is the description of a time-dependent chemical potential by an effective electron distribution. While this yields the correct expression (80) for the dc current, it does not capture the interference terms in the noise formula (81). This reveals that a Tien-Gordon-like approach yields the correct dc current while for the noise (and other higher-order correlation functions) it is only valid in a high-frequency limit.

For large voltages where  $f_L = 0$  and  $f_R = 1$ , the sums over the Fourier coefficients in Eqs. (80) and (81) can be evaluated with the help of the sum rule  $\sum_{k'} a_{k'}^* a_{k'+k} = \delta_{k,0}$ . Then both the dc current and the zero-frequency noise become identical to their value in the absence of the

driving. This means that for a sufficiently large transport voltage, a time-dependent gate voltage has no influence on the average current and the zero-frequency noise.

### E. High-frequency driving

Many effects occurring in driven quantum systems, such as coherent destruction of tunneling<sup>24</sup> or current and noise control,<sup>29,30</sup> are most pronounced for large excitation frequencies. Thus, it is particularly interesting to derive for the present Floquet approach an expansion in terms of  $1/\Omega$ . Thereby, the driven system will be approximated by a static system with renormalized parameters. Such a perturbation scheme has been developed for two-level systems in Ref. 53 and applied to driven tunneling in bistable systems<sup>65</sup> and superlattices.<sup>26</sup> For open quantum system, the coupling to the external degrees of freedom (e.g., the leads or a heat bath) bears additional complications that have been solved heuristically in Ref. 44 by replacing the Fermi functions by effective electron distributions. In the following, we present a rigorous derivation of this approach based on a perturbation theory for the Floquet equation (55).

We assume a driving that leaves all off-diagonal matrix elements of the wire Hamiltonian time-independent while the tight-binding levels undergo a position-dependent, time-periodic driving  $f_n(t) = f_n(t + \mathcal{T})$  with zero time-average. Then, the wire Hamiltonian is of the form

$$\mathcal{H}_{\text{wire}}(t) = \mathcal{H}_0 + \sum_n f_n(t) |n\rangle\langle n|. \quad (82)$$

If  $\hbar\Omega$  represents the largest energy scale of the problem, we can in the Floquet equation (55) treat the *static* part of the Hamiltonian as a perturbation. Correspondingly, the eigenfunctions of the operator  $\sum_n f_n(t) |n\rangle\langle n| - i\hbar d/dt$  determine the zeroth order Floquet states

$$e^{-iF_n(t)} |n\rangle. \quad (83)$$

We have defined the function

$$F_n(t) = \frac{1}{\hbar} \int_0^t dt' f_n(t') = F_n(t + \mathcal{T}), \quad (84)$$

which is  $\mathcal{T}$ -periodic due to the zero time-average of  $f_n(t)$ . As a consequence of this periodicity, to zeroth order the quasienergies are zero (mod  $\hbar\Omega$ ) and the Floquet spectrum is given by multiples of the photon energy,  $k\hbar\Omega$ . Each  $k = 0, \pm 1, \pm 2, \dots$  defines a degenerate subspace of the extended Hilbert space. If now  $\hbar\Omega$  is larger than all other energy scales, the first-order correction to the Floquet states and the quasienergies can be calculated by diagonalizing the perturbation in the subspace defined by  $k = 0$ . Thus, we have to solve the time-independent eigenvalue equation

$$(\mathcal{H}_{\text{eff}} - i\Sigma)|\alpha\rangle = (\epsilon_\alpha^1 - i\hbar\gamma_\alpha^1)|\alpha\rangle. \quad (85)$$

The time-independent effective Hamiltonian  $\mathcal{H}_{\text{eff}}$  is defined by the matrix elements of the original static Hamiltonian  $\mathcal{H}_0$  with the zeroth order Floquet states (83),

$$(\mathcal{H}_{\text{eff}})_{nn'} = \int_0^{\mathcal{T}} \frac{dt}{\mathcal{T}} e^{iF_n(t)} (\mathcal{H}_0)_{nn'} e^{-iF_{n'}(t)}. \quad (86)$$

The  $t$ -integration constitutes the inner product in the Hilbert space extended by a periodic time coordinate.<sup>54</sup> To first order in  $1/\Omega$ , the quasienergies  $\epsilon_\alpha^1 - i\hbar\gamma_\alpha^1$  are given by the eigenvalues of the static equation (85) and, consequently, the corresponding Floquet states read

$$|u_\alpha(t)\rangle = \sum_n e^{-iF_n(t)} |n\rangle\langle n|\alpha\rangle. \quad (87)$$

The fact that all  $F_n(t)$  are  $\mathcal{T}$ -periodic, allows to write in (87) the time-dependent phase factor as a Fourier series,

$$e^{-iF_n(t)} = \sum_k a_{n,k} e^{-ik\Omega t}. \quad (88)$$

Thus,  $\langle n|u_{\alpha,k}\rangle = a_{n,k}\langle n|\alpha\rangle$  and the Green function for the high-frequency driving reads

$$G_{nn'}^{(k)}(\epsilon) = \sum_{k'} a_{n,k'+k} a_{n',k'}^* G_{nn'}^{\text{eff}}(\epsilon - k'\hbar\Omega), \quad (89)$$

where  $G^{\text{eff}}(\epsilon)$  denotes the Green function corresponding to the static Hamiltonian  $\mathcal{H}_{\text{eff}}$  with the self-energy  $\Sigma$ . Finally, substituting  $\epsilon \rightarrow \epsilon + k'\hbar\Omega$  and using the sum rule  $\sum_{k'} a_{n,k'+k} a_{n',k'}^* = \delta_{k,0}$ , we obtain

$$\bar{I} = \frac{e}{\hbar} \int d\epsilon T_{\text{eff}}(\epsilon) \{f_{R,\text{eff}}(\epsilon) - f_{L,\text{eff}}(\epsilon)\}. \quad (90)$$

The effective transmission  $T_{\text{eff}}(\epsilon) = \Gamma_L \Gamma_R |G_{1N}^{\text{eff}}(\epsilon)|^2$  is computed from the effective Hamiltonian (86); the electron distribution is given by

$$f_{L,\text{eff}}(\epsilon) = \sum_k |a_{1,k}|^2 f_L(\epsilon + k\hbar\Omega) \quad (91)$$

and  $f_{R,\text{eff}}$  follows from the replacement  $(1, L) \rightarrow (N, R)$ .

In order to derive a high-frequency approximation for the zero-frequency noise  $\bar{S}$ , we insert the Green function (89) into (45) and neglect products of the type  $G^{\text{eff}}(\epsilon - k\hbar\Omega) G^{\text{eff}}(\epsilon - k'\hbar\Omega)$  for  $k \neq k'$ . Employing the above sum rule for the Fourier coefficients  $a_{n,k}$ , we obtain for the noise the static expression (62) but with the transmission  $T(\epsilon)$  and the Fermi functions  $f_{R,L}(\epsilon)$  replaced by the effective transmission  $T_{\text{eff}}(\epsilon)$  and the effective distribution function (91), respectively. The fact that  $f_{L,\text{eff}}(\epsilon)$  is generally not a mere Heaviside step function has an intriguing consequence: In the presence of driving, the noise remains finite even if both voltage and temperature are zero.

Two differences between the high-frequency approximation and the homogeneous driving, cf. Sec. IV D, are

worth mentioning: First, the static transmission is now replaced by an effective transmission which can be considerably influenced by the driving, see below. Second, in general  $a_{1,k} \neq a_{N,k}$  such that  $f_{R,\text{eff}} \neq f_{L,\text{eff}}$ . This means that the driving can create an effective bias and thereby create a non-adiabatic pump current. By contrast Eq. (80) reveals that a homogeneous driving cannot create such a pump current. Moreover, if all  $F_n$  are identical as in the case of a homogeneous driving, the effective Hamiltonian  $\mathcal{H}_{\text{eff}}$  equals the original static Hamiltonian. Then, also the second line of Eq. (81) can be written in terms of the static transmission  $T(\epsilon)$ .

## V. CONDUCTOR DRIVEN BY AN OSCILLATING DIPOLE FIELD

In this section, we apply the formalism derived in Secs. III and IV to study the conduction and noise properties of a nanoscale conductor under the influence of an electromagnetic field. As an elementary model that captures the essential features of a molecular wire,<sup>6</sup> we employ a tight-binding model composed of  $N$  sites as sketched in Fig. 1. Each orbital is coupled to its nearest neighbor by a hopping matrix element  $\Delta$ , thus, the single-particle wire Hamiltonian reads

$$\mathcal{H}_{\text{wire}}(t) = -\Delta \sum_{n=1}^{N-1} (|n\rangle\langle n+1| + |n+1\rangle\langle n|) + \sum_n [E_n + f_n(t)] |n\rangle\langle n|, \quad (92)$$

where  $E_n$  denote the on-site energies of the tight-binding levels. Within a dipole approximation, the oscillating electromagnetic field causes the time-dependent level shifts

$$f_n(t) = A \cos(\Omega t) x_n \quad (93)$$

with  $x_n = (N + 1 - 2n)/2$  the scaled position of site  $|n\rangle$ . Since typical laser frequencies are below the work function of a usual metal, we assume that the radiation does not penetrate the leads and that, consequently, the leads stay in thermal equilibrium. The energy  $A$  denotes the electrical field amplitude multiplied by the electron charge and the distance between two neighboring sites and, thus, depends implicitly on the length of the sample. This model describes, as well, an array of coherently coupled quantum dots<sup>1,2,3</sup> under the influence of microwave radiation.

The dipole approximation inherent to the driving (93) neglects the propagation of the electromagnetic field and, thus, is valid only for wavelengths that are much larger than the size of the sample.<sup>66</sup> This condition is indeed fulfilled for both applications we have in mind: For molecular wires, we consider frequencies up to the optical spectral range, i.e., wavelengths of the order  $1\mu\text{m}$  and samples that extend over a few nanometers. Coupled quantum

dots typically<sup>1,2,3</sup> have a distance of less than  $1\mu\text{m}$  while the coupling matrix element  $\Delta$  is of the order of  $30\mu\text{eV}$  which corresponds to a wavelength of roughly  $1\text{cm}$ .

We assume that the wire couples equally strong to both leads, thus,  $\Gamma_L = \Gamma_R \equiv \Gamma$ . An applied transport voltage  $V$  is mapped to a symmetric shift of the leads' chemical potentials,  $\mu_R = -\mu_L = eV/2$ . Moreover, for the evaluation of the dc current and the zero-frequency noise, we restrict ourselves to zero temperature. The zero-temperature limit is physically well justified for molecular wires at room temperature and for quantum dots at helium temperature since in both cases thermal electron excitations do not play a significant role.

### A. Current and noise suppression

For a wire described by the Hamiltonian (92), it has been found<sup>30</sup> that a dipole force of the form (93) suppresses the transport if the ratio  $A/\hbar\Omega$  is close to a zero of the Bessel function  $J_0$  (i.e., values 2.405..., 5.520..., 8.654..., ...). Moreover, in the vicinity of such suppressions, the shot noise characterized by the Fano factor (13) assumes two characteristic minima. These suppression effects are most pronounced in the high-frequency regime, i.e., if the energy quanta  $\hbar\Omega$  of the driving exceed the energy scales of the wire. Thus, before going into a detailed discussion, we start with a qualitative description of the effect based on the static approximation for a high-frequency driving that has been derived in Sec. IV E.

Let us consider first the limit of a voltage which is so large that in Eq. (90),  $f_{R,\text{eff}} - f_{L,\text{eff}}$  can be replaced by unity. Then, the average current is determined by the effective Hamiltonian

$$\mathcal{H}_{\text{eff}} = -\Delta_{\text{eff}} \sum_{n=1}^{N-1} (|n\rangle\langle n+1| + |n+1\rangle\langle n|) + \sum_{n=1}^N E_n |n\rangle\langle n|, \quad (94)$$

which has been derived by inserting the driving (93) into Eqs. (84) and (86). Then, obviously  $\mathcal{H}_{\text{eff}}$  is identical to the Hamiltonian (92) in the absence of the driving field but with the tunnel matrix element renormalized according to

$$\Delta \rightarrow \Delta_{\text{eff}} = J_0(A/\hbar\Omega)\Delta. \quad (95)$$

Since the Bessel function  $J_0$  assumes values between zero and one, the amplitude of the driving field allows to switch the absolute value of the effective hopping on the wire,  $\Delta_{\text{eff}}$ , between 0 and  $\Delta$ . Since the transmission of an undriven wire is proportional to  $|\Delta|^2$ , the effective transmission  $T_{\text{eff}}(\epsilon)$  acquires a factor  $J_0^2(A/\hbar\Omega)$ . This renormalization of the hopping results finally in a current suppression.<sup>29,30</sup>

For the discussion of the shot noise, we employ the Fano factor (13) as a measure. In the limit of large applied voltages, we have to distinguish two limits: (i) weak wire-lead coupling  $\Gamma \ll \Delta_{\text{eff}}$  (i.e., weak with respect to the effective hopping) and (ii) strong wire-lead

coupling  $\Gamma \gg \Delta_{\text{eff}}$ . In the first case, the tunnel contacts between the lead and the wire act as “bottlenecks” for the transport. In that sense they form barriers. Thus qualitatively, we face a double barrier situation and, consequently, expect the shot noise to exhibit a Fano factor  $F \approx 1/2$ .<sup>33</sup> In the second case, the links between the wire sites act as  $N - 1$  barriers. Correspondingly, the Fano factor assumes values  $F \approx 1$  for  $N = 2$  (single barrier) and  $F \approx 1/2$  for  $N = 3$  (double barrier)<sup>67</sup>. At the crossover between the two limits, the conductor is optimally “barrier free” such that the Fano factor assumes its minimum.

In order to be more quantitative, we evaluate the current and the zero-frequency noise in more detail thereby considering a finite voltage. This requires a closer look at the effective electron distribution (91); in particular, we have to quantify the concept of a “practically infinite” voltage. In a static situation, the voltage can be replaced by infinity,  $f_R(\epsilon) = 1 = 1 - f_L(\epsilon)$ , if all eigenenergies of the wire lie well inside the range  $[\mu_L, \mu_R]$ . In contrast to the Fermi functions, the effective electron distribution (91) which is decisive here, decays over a broad range in multiple steps of size  $\hbar\Omega$ . Since for our model,  $T_{\text{eff}}(\epsilon)$  is peaked around  $\epsilon = 0$ , we replace here the effective electron distributions by their values for  $\epsilon = 0$ ,

$$f_{\ell, \text{eff}}(0) = \sum_{k < \mu_{\ell}/\hbar\Omega} J_k^2\left(\frac{A(N-1)}{2\hbar\Omega}\right), \quad (96)$$

for zero temperature. We have inserted the coefficients  $a_{1,k} = J_k(A(N-1)/2\hbar\Omega)$  and  $a_{N,k} = J_{-k}(A(N-1)/2\hbar\Omega)$  which have been computed directly from their definition (88);  $J_k$  denotes the  $k$ th order Bessel functions of the first kind. The current, the noise, and the Fano factor are given by the static expressions (60) and (62) with the transmission and the electron distribution replaced by the corresponding effective quantities,  $T_{\text{eff}}$  and  $f_{\text{eff},\ell}$ , respectively. Thus, we obtain

$$\bar{I} = \lambda \bar{I}_{\infty}, \quad (97)$$

$$\bar{S} = \lambda^2 \bar{S}_{\infty} + \frac{e}{2}(1 - \lambda^2)\bar{I}_{\infty}, \quad (98)$$

$$F = \lambda F_{\infty} + \frac{1 - \lambda^2}{2\lambda}, \quad (99)$$

respectively, where the subscript  $\infty$  denotes the corresponding quantities in the infinite voltage limit,

$$\bar{I}_{\infty} = \frac{e}{h} \int d\epsilon T_{\text{eff}}(\epsilon), \quad (100)$$

$$\bar{S}_{\infty} = \frac{e^2}{h} \int d\epsilon T_{\text{eff}}(\epsilon)[1 - T_{\text{eff}}(\epsilon)], \quad (101)$$

and  $F_{\infty} = \bar{S}_{\infty}/e\bar{I}_{\infty}$ . The factor

$$\lambda = f_{R, \text{eff}}(0) - f_{L, \text{eff}}(0) = \sum_{|k| \leq K(V)} J_k^2\left(\frac{A(N-1)}{2\hbar\Omega}\right) \quad (102)$$

reflects the influence of a finite voltage;  $K(V)$  denotes the largest integer not exceeding  $e|V|/2\hbar\Omega$ . Since  $J_k(x) \approx 0$  for  $|k| > x$  and  $\sum_k J_k^2(x) \approx 1$ , we find  $\lambda = 1$  if  $K(V) > A(N-1)/2\hbar\Omega$ . This means that for small driving amplitudes  $A < eV/(N-1)$ , we can consider the voltage as practically infinite. With an increasing driving strength,  $\lambda$  decreases and, thus, the current becomes smaller by a factor  $\lambda$  but still exhibits suppressions. By contrast, since  $F_{\infty} \leq 1$  for all situations considered here [cf. the remark after Eq. (64)], we find from Eq. (99) that the Fano factor will increase with smaller  $\lambda$ .

## B. Numerical results

The qualitative discussion of the current and noise suppressions can be corroborated by exact numerical results. For this purpose, we have solved numerically the Floquet equation (55). With the resulting Floquet states and quasienergies, we obtained the Green function (58). In the zero temperature limit considered here, the Fermi functions in the expressions for the average current (37) and the zero-frequency noise (45) become step functions. The remaining energy integrals can be performed analytically since the integrands are rational functions.

### 1. Intermediate wire-lead coupling

Figure 2 depicts the average current, the zero-frequency noise, and the corresponding Fano factor for a wire that consists of  $N = 3$  sites with on-site energies  $E_n = 0$  as sketched in Fig. 1. The driving frequency  $\Omega = 5\Delta/\hbar$  lies above all transition energies of the wire states and the applied voltage  $V = 48\Delta/e$  is relatively large. This particular value of the voltage has been selected to avoid chemical potentials to lie close to multiples of  $\hbar\Omega$ , i.e., close to the steps of the effective electron distribution (96). The wire-lead coupling  $\Gamma = 0.5\Delta$  is sufficiently weak, such that in the absence of the driving, the transport is dominated by resonant tunneling. Correspondingly, the current is essentially determined by the hopping rate  $\Gamma/2\hbar$  of the electrons from the lead to the wire. The noise exhibits a Fano factor  $F \approx 1/2$  which is the characteristic value for the transport across a double barrier.<sup>33,68</sup> With an increasing driving amplitude, the current becomes smaller until it reaches its minimum when the ratio  $A/\hbar\Omega$  assumes a zero of the Bessel function  $J_0$ . Note that while the analytical treatment within a high-frequency approximation predicts a vanishing current, the exact result is still roughly 1% of the value in the absence of the driving. Close to the current suppression, the effective tunnel matrix element (95) is much smaller than the wire-lead coupling  $\Gamma$  and the connections to the central site of the wire form a double barrier. Consequently, we again find a Fano factor  $F \approx 1/2$ . At the crossover  $\Delta_{\text{eff}} \approx \Gamma$ , the effective barriers vanish and, therefore, the Fano factor assumes its minimum.

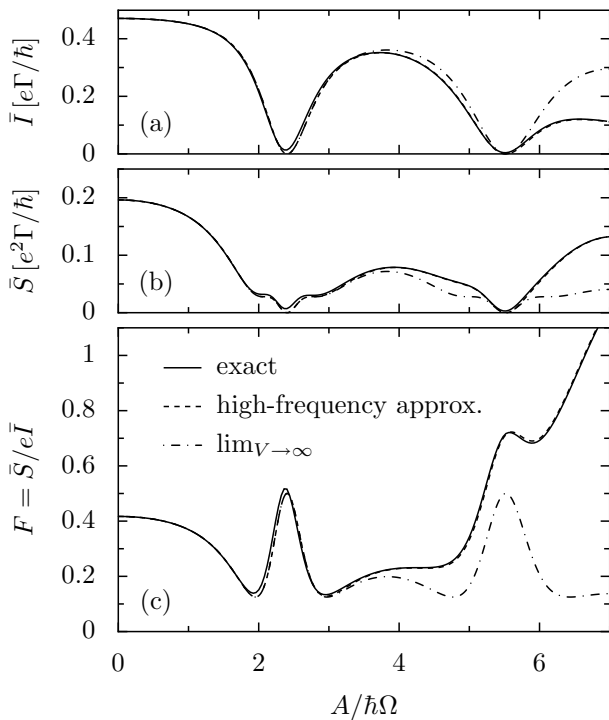


FIG. 2: Time-averaged current (a), zero-frequency noise (b), and Fano factor (c) for a conductor consisting of  $N = 3$  sites with equal on-site energies,  $E_n = 0$ , as a functions of the driving amplitude  $A$ . The driving frequency is  $\Omega = 5\Delta/\hbar$ , the wire-lead coupling is  $\Gamma = 0.5\Delta$ , and the chemical potentials are  $\mu_R = -\mu_L = 24\Delta$ . The exact numerical results (solid lines) are compared to the high-frequency approximation for finite (dashed) and infinite voltage (dash-dotted).

These exact numerical results are well reproduced by the expressions (97)–(99) obtained within a high-frequency approximations for finite voltage. Figure 2 also reveals that for small driving amplitudes,  $A < eV/(N - 1)$ , the assumption of a practically infinite voltage yields the correct results. By contrast, for larger driving amplitudes,  $A > eV/(N - 1)$ , the Fano factor can assume values  $F > 1$ , i.e., the shot noise becomes even larger than in the static situation.

As the coupling strength  $\Gamma$  is lowered, the distance between a pair of minima of the Fano factor becomes smaller until the minima finally vanish<sup>30</sup> (not shown). In this limit, the current and the noise are given by the weak coupling results (74) and (75), respectively. The corresponding Fano factor  $F = 1/2$  [cf. the discussion after Eq. (75)] is independent of the driving amplitude.

Figure 3a depicts the behavior for a driving frequency which is of the order of the wire excitations,  $\Omega = \Delta/\hbar$ . Then, the high-frequency approximation is no longer applicable. Nevertheless, the average current exhibits clear minima with a reduction of the order 50%. Compared to the high-frequency case, these minima are shifted towards smaller driving amplitudes, i.e., they occur for ratios  $A/\hbar\Omega$  slightly below the zeros of the Bessel function

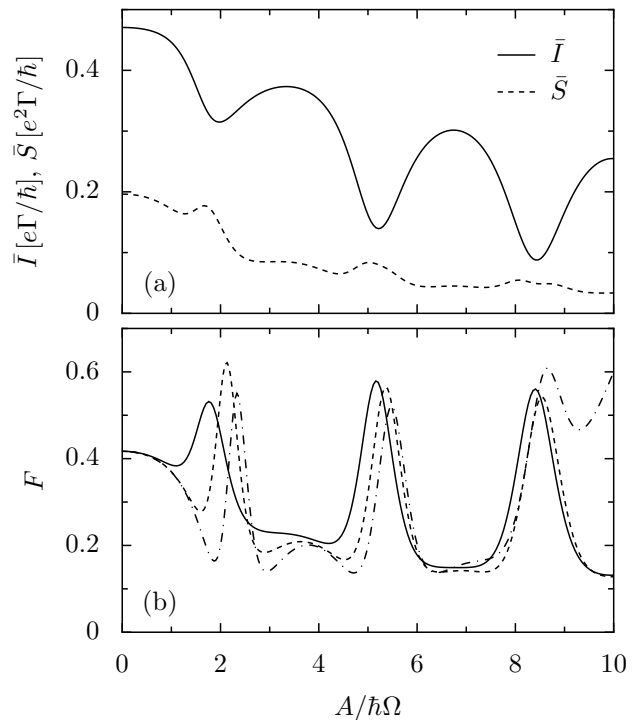


FIG. 3: (a) Time-averaged current (solid line) and zero-frequency noise (dashed line) as a function of the driving amplitude for the driving frequency  $\Omega = \Delta/\hbar$ . (b) Corresponding Fano factor for the same data (solid line) and for the driving frequencies  $\Omega = 1.5\Delta/\hbar$  (broken) and  $\Omega = 3\Delta/\hbar$  (dash-dotted). All other parameters are as in Fig. 2.

$J_0$ . At the minima of the current, the Fano factor (solid line in Fig. 3b) still assumes a maximum with a value close to  $F \approx 1/2$ . Although, the sharp minima close to the current suppressions have vanished, in-between the maxima the Fano factor assumes remarkably low values ( $F \approx 0.2$ ). Figure 3b also reveals that already for  $\Omega \approx 3\Delta/\hbar$ , the high-frequency regime is reached.

## 2. Strong wire-lead coupling

For strong wire-lead coupling, it is possible to choose a driving frequency that is large with respect to the wire excitations, but small as compared to the coupling  $\Gamma$ , thus  $\Delta \ll \hbar\Omega \ll \Gamma$ . Figure 4 depicts the current and the Fano factor in this limit for wires with a different number of sites. The qualitative difference between these cases can be explained by the fact that due to the strong coupling, the first and the last wire site hybridize with the leads. Then the setup behaves similar to a wire with  $N - 2$  sites and a weak wire-lead coupling  $\propto \Delta^2/\Gamma$ . This means that for  $N = 2$  the wire acts as point contact while for  $N = 3$ , we qualitatively have resonant transport through a single level. In both cases remains no tunneling matrix element of the wire that could be renormalized and, consequently, for  $N \leq 3$  the current suppressions vanish in

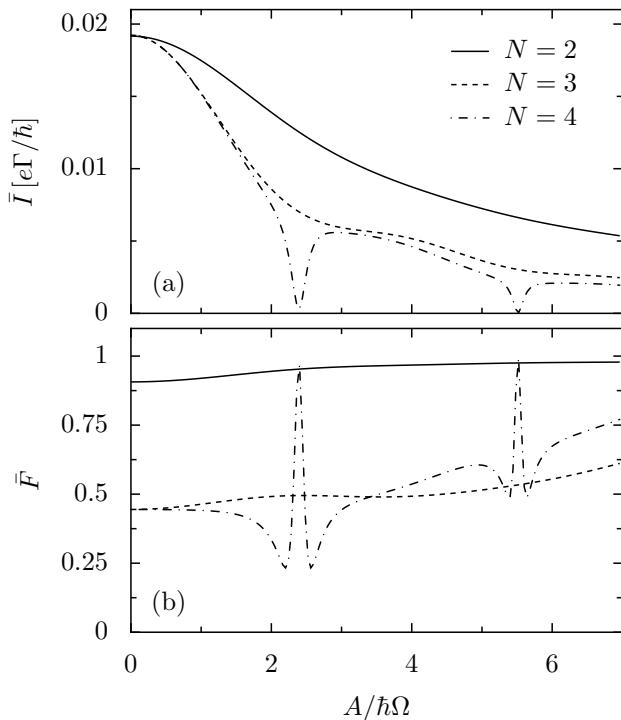


FIG. 4: Time-averaged current (a) and Fano factor (b) as a function of the driving amplitude  $A$  for a wire with  $N = 2, 3, 4$  sites and the wire-lead coupling strength  $\Gamma = 10\Delta$ . The other parameters are  $E_n = 0$ ,  $\Omega = 5\Delta/\hbar$  and  $\mu_R = -\mu_L = 25\Delta$ .

the strong-coupling limit (cf. Fig. 4a). This scenario is also reflected in the behavior of the Fano factor (Fig. 4b) which exhibits the characteristic values  $F \approx 1$  (point contact) for  $N = 2$  and  $F \approx 1/2$  (single resonant level) for  $N = 3$ . Finally, for  $N = 4$  we observe the behavior of a driven wire with two sites and weak coupling.<sup>44</sup> Then, a vanishing effective hopping  $\Delta_{\text{eff}} \approx 0$  corresponds to a point contact, thus,  $F \approx 1$ . Although the behavior of the Fano factor can be explained by drawing analogies to a weakly coupled wire with  $N - 2$  sites, the global decay of the current with the driving amplitude, cf. Fig. 4a, is not within the scope of this intuitive picture.

### 3. Internal bias

So far, we have assumed that all on-site energies of the wire are identical. In an experimental setup, however, the applied transport voltage acts also a static dipole force which rearranges the charge distribution in the conductor and thereby causes an internal potential profile.<sup>69,70,71</sup> The self-consistent treatment of such effects is, in particular in the time-dependent case, rather ambitious and beyond the scope of this work. Thus, here we only derive the consequences of a static bias without determining its shape from microscopic considerations. We assume a position-dependent static shift of the on-site energies by

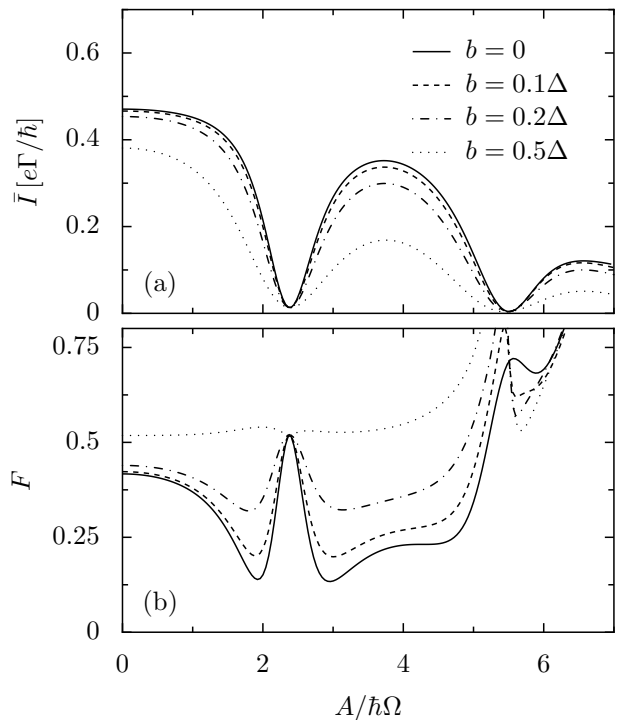


FIG. 5: Time-averaged current (a) and Fano factor (b) as a function of the driving amplitude  $A$  for a wire with  $N = 3$  sites in the presence of an internal bias. The on-site energies are  $E_1 = b$ ,  $E_2 = 0$ ,  $E_3 = -b$ . All other parameters are as in Fig. 2.

an energy  $-b x_n$ , i.e., for a wire with  $N = 3$  sites,

$$E_1 = b, \quad E_2 = 0, \quad E_3 = -b. \quad (103)$$

Figure 5a demonstrates that the behavior of the average current is fairly stable against the bias. In particular, we still find pronounced current suppressions. Note that since  $b \ll \Omega$  a high-frequency approximation is still possible. As a main effect of the bias, we find reduced current maxima while the minima remain. By contrast, the minima of the Fano factor (Fig. 5b) become washed out: Once the bias becomes of the order of the wire-lead coupling,  $b \approx \Gamma$ , the structure in the Fano factor vanishes and we find  $F \approx 1/2$  for all driving amplitudes  $A < eV/(N - 1)$  [cf. the discussion after Eq. (102)]. Interestingly, the value of the Fano factor at current suppressions is bias independent.

## VI. CONCLUSIONS

We have derived with Eqs. (37)–(39), (40), and (45) expressions for the dc current, the zero-frequency noise, and the time-dependent current for the electron transport through ac-driven nanoscale systems. A cornerstone of our approach is the relation of the propagator to a non-Hermitian Floquet equation. This yields

explicit formulae for the current and the noise. Moreover, the connection to Floquet theory allows to elucidate various approximation schemes that enable an efficient computation and, in addition, provide physical insight. Above all, a high-frequency approximation has emerged to be very useful: Within an expansion in  $1/\Omega$ , the driven transport problem can be approximated by a time-independent transport problem with a renormalized tunneling and effective distribution functions for the lead electrons. The conductance properties of the latter can be derived with standard methods. Moreover, for the case of a time-dependent gating voltage, we have revealed the limitations of the Tien-Gordon approach: While such a treatment provides the correct expression for the current, it neglects interferences of different Floquet channels.

A detailed investigation of the recently found shot noise suppression provided a deeper understanding of this effect. In particular, the analytical treatment within a high-frequency approximation can explain the characteristic emergence of the current suppressions which are accompanied by a noise maximum and two remarkably low minima. A numerical study fully confirmed the analytical results. For lower driving frequencies, i.e., beyond the high-frequency limit, the current suppressions become considerably less pronounced. By contrast, the shot noise suppression turned out to be more stable. Thus, since the current stays remarkably large while the noise is controllable, this regime is particularly promising for applications. At first sight, in the limit of strong wire-lead coupling these phenomena appear quite different. A closer look, however, revealed that the strong coupling entails a hybridization of the first and the last site with the respective lead. Therefore, the wire behaves qualitatively like a weakly coupled wire with two sites less. Moreover, we have found that the noise suppressions are quite sensitive to an internal bias. Once the on-site energies of neighboring sites have differences of the order of the wire-lead coupling energy, the minima of the Fano factor vanish. A most interesting application of these results is the development of current sources with a controllable noise level.

### Acknowledgments

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### APPENDIX A: AC TRANSPORT VOLTAGE

Within this work, we focus on models where the driving enters solely by means of time-dependent matrix elements of the wire Hamiltonian while the leads and the wire-lead couplings remain time-independent. An *a priori* different type of driving is the application of a time-dependent transport voltage. In this appendix, we demonstrate that a setup with an oscillating transport voltage can be mapped by a gauge transformation to a Hamiltonian of the form (1). Consequently, it is possible to apply the formalism derived in Sec. III also to situations with an oscillating transport voltage.

We restrict the discussion to the case where the electron energies of only the left lead are modified by an external  $\mathcal{T}$ -periodic voltage  $V_{ac}(t)$  with zero time-average, thus in the left lead

$$\epsilon_q \rightarrow \epsilon_q - eV_{ac}(t). \quad (A1)$$

The generalization to a situation where also the levels in the right lead are  $\mathcal{T}$ -periodically time-dependent, is straightforward. Since an externally applied voltage causes a potential drop along the wire,<sup>69,70,71</sup> we have to assume for consistency that for an ac voltage, the wire Hamiltonian also obeys a time-dependence. Ignoring such a time-dependent potential profile enables a treatment of the transport problem within the approach of Refs. 63 and 64. In the general case, however, we have to resort to the approach put forward with this work.

We start out by a gauge transformation of the Hamiltonian (1) with the unitary operator

$$U_{ac}(t) = \exp \left\{ -i\phi(t) \left( c_1^\dagger c_1 + \sum_q c_{Lq}^\dagger c_{Lq} \right) \right\} \quad (A2)$$

where

$$\phi(t) = -\frac{e}{\hbar} \int^t dt' V_{ac}(t') \quad (A3)$$

describes the phase accumulated from the oscillating voltage. The transformation (A2) has been constructed such that the new Hamiltonian  $\tilde{H}(t) = U_{ac}^\dagger H(t) U_{ac} - i\hbar U_{ac}^\dagger \dot{U}_{ac}$  possesses a time-independent tunnel coupling. Since, the operator  $c_1$  transforms as  $c_1 \rightarrow c_1 \exp(-i\phi(t))$ , the matrix elements  $H_{nn'}(t)$  of the wire Hamiltonian acquire an additional time-dependence,

$$H_{nn'}(t) \rightarrow \tilde{H}_{nn'}(t) = H_{nn'}(t) e^{-i\phi(t)(\delta_{n'1} - \delta_{n1})} + eV_{ac}(t) \delta_{n1} \delta_{n'1}. \quad (A4)$$

The second term in the Hamiltonian (A4) stems from  $-i\hbar U_{ac}^\dagger \dot{U}_{ac}$ . Owing to the zero time-average of the voltage  $V_{ac}(t)$ , the phase  $\phi(t)$  is  $\mathcal{T}$ -periodic. Therefore, the transformed wire Hamiltonian is also  $\mathcal{T}$ -periodic while the contact and the lead contributions are time-independent, thus,  $\tilde{H}(t)$  is of form (1).



## APPENDIX B: ALTERNATIVE DERIVATION

In Ref. 30, the expressions (37) and (45) for the current and the noise in the wide-band limit have been derived by eliminating the leads in favor of a stochastic operator. In this appendix, we detail this approach. Like in Section III, we start here also from the Heisenberg equations (14)–(16) for the annihilation operators. The ones for the lead operators, Eq. (14), are easily integrated to read

$$c_{Lq}(t) = c_{Lq}(t_0)e^{-i\epsilon_q(t-t_0)/\hbar} - \frac{iV_{Lq}}{\hbar} \int_0^{t-t_0} d\tau e^{-i\epsilon_q\tau/\hbar} c_1(t-\tau) \quad (\text{B1})$$

and  $c_{Rq}(t)$  accordingly. Inserting (B1) into the Heisenberg equations (15) for the wire operators yields

$$\begin{aligned} \dot{c}_{1/N} &= -\frac{i}{\hbar} \sum_{n'} H_{1/N,n'}(t) c_{n'} - \frac{\Gamma_{L/R}}{2\hbar} c_{1/N} + \xi_{L/R}(t), \\ \dot{c}_n &= -\frac{i}{\hbar} \sum_{n'} H_{nn'}(t) c_{n'}, \quad n = 2, \dots, N-1. \end{aligned} \quad (\text{B2})$$

Owing to the wide-band limit, the dissipative terms are memory free. Within the chosen grand canonical ensembles the operator-valued Gaussian noise  $\xi_\ell(t) = -(i/\hbar) \sum_q V_{\ell q}^* e^{-i\epsilon_q(t-t_0)/\hbar} c_{\ell q}(t_0)$  obeys

$$\langle \xi_\ell(t) \rangle = 0, \quad (\text{B3})$$

$$\langle \xi_\ell^\dagger(t) \xi_{\ell'}(t') \rangle = \delta_{\ell\ell'} \frac{\Gamma_\ell}{2\pi\hbar^2} \int d\epsilon e^{i\epsilon(t-t')/\hbar} f_\ell(\epsilon). \quad (\text{B4})$$

The current operator then assumes the form

$$I_L(t) = \frac{e}{\hbar} \Gamma_L c_1^\dagger(t) c_1(t) - e \{ c_1^\dagger(t) \xi_L(t) + \xi_L^\dagger(t) c_1(t) \}. \quad (\text{B5})$$

The homogeneous set of equations that corresponds to (B2) coincides with the equations of motion (46) and (50) which are solved by the Floquet states  $|u_\alpha(t)\rangle$ . Thus, the Floquet states  $|u_\alpha(t)\rangle$  together with the adjoint states

$|u_\alpha^\dagger(t)\rangle$ , allow to write the solution of (B2) in closed form. In the asymptotic limit  $t_0 \rightarrow -\infty$ , it reads

$$c_n(t) = \int_0^\infty d\tau \langle n | U(t, t-\tau) \times \{ |1\rangle \xi_L(t-\tau) + |N\rangle \xi_R(t-\tau) \} \}. \quad (\text{B6})$$

where  $U(t, t-\tau)$  is the propagator (56) for the wire electrons.

To obtain the current  $\langle I_L(t) \rangle$ , we insert the operator (B6) into the expression (40) and use the expectation values (B4). With the Green function (32), we find the still unsymmetric expression

$$\begin{aligned} \langle I_L(t) \rangle &= \frac{e\Gamma_L}{2\pi\hbar} \int d\epsilon \left\{ \Gamma_L |G_{11}(t, \epsilon)|^2 f_L(\epsilon) \right. \\ &\quad \left. + \Gamma_R |G_{1N}(t, \epsilon)|^2 f_R(\epsilon) \right. \\ &\quad \left. + i[G_{11}^*(t, \epsilon) - G_{11}(t, \epsilon)] f_L(\epsilon) \right\}. \end{aligned} \quad (\text{B7})$$

For a symmetrization, we eliminate the backscattering terms, i.e., terms containing  $G_{11}$ , by use of the relation<sup>38</sup>

$$G^\dagger(t, \epsilon) - G(t, \epsilon) = i\hbar \frac{d}{dt} G^\dagger(t, \epsilon) G(t, \epsilon) + 2iG^\dagger(t, \epsilon) \Sigma G(t, \epsilon) \quad (\text{B8})$$

which follows readily from the Floquet representation (56) of the propagator and the Floquet eigenvalue equation (55) together with its adjoint. A subsequent Fourier transformation with respect to  $\tau = t - t'$  yields Eq. (B8). By inserting the matrix element  $\langle 1 | \dots | 1 \rangle$ , we obtain from (B7) for the time-dependent current the symmetric expression (40).

To derive an expression for the zero frequency noise, we insert the operator (B6) into the definition (9) of the current-current correlation function and integrate over the times  $\tau$  and  $t$ . Again, we employ the relation (B8) to bring  $S$  into the symmetric form (45).

\* New address: Laboratoire de Physique, Ecole normale supérieure de Lyon, 46, Allée d'Italie, 69364 Lyon Cedex 07, France

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